

NEANSC WORKING PARTY ON INTERNATIONAL EVALUATION COOPERATION

SUBGROUP 12: NUCLEAR MODEL VALIDATION

REPORT FROM THE 1-ST MEETING  
OF SUBGROUP 12  
ON  
NUCLEAR MODEL VALIDATION  
Gatlinburg May 8, 1994

G.Reffo  
May 30, 1994

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Introduction

At the 5-th meeting of the NEANSC working party on International Evaluation Cooperation (IEC), held at Aix-en-Provence, France, 16-th and 17-th June 1993, new subgroup activities have been established, one of which is subgroup 12 on NUCLEAR MODEL VALIDATION (NMV) (Monitor: C. Dunford, subsequently replaced by P. Oblozinsky; Coordinator: G. Reffo).

According to the intentions of the International Evaluation Working Party [ as outlined in the document NEA/NSC/WPEC(93)2, IEC-80 ], subgroup 12, will:

- \*\*\*  
coordinate the collection of nuclear models,
- \*\*\*  
indicate the range of applicability of each,
- \*\*\*  
produce a well-tested transportable system of computer programs to be used by the nuclear data community,
- \*\*\*  
document all the mentioned activities,
- \*\*\*  
cooperate closely with the IAEA coordinated development of a data base of nuclear model parameters.

# 1. NEED FOR NUCLEAR MODEL VALIDATION AND INTERNATIONAL COOPERATION FRAMEWORK.

## 1.1 Hystorical background and the present situation.

Low and intermediate energy nuclear physics has become a mature science and is well oriented for applications. Scientific developments in the field of both pure and applied physics are demanding nuclear data of higher and higher quality in an increasing range of masses, of reaction-types and of energies.

In the past, the bulk of nuclear data needed for technological applications was mainly provided by experimental measurement programmes. With increasing computer capabilities and availability, theoretical developments of nuclear physics have been greatly facilitated so that we start having available nuclear models and codes, as well as nuclear modelling methodologies, allowing the production of reliable nuclear data at a cost uncomparably lower than measurements.

The trend of declining funding for low and intermediate energy nuclear physics has particularly affected measurements activities, and there does not seem to be any prospect of change in the foreseeable future. It will never be possible, however, to rely completely, solely, on theoretical model predictions, this is why one has to strongly support some experimental activities. Even a few measurements, in fact, could be sufficient to benchmark model assumptions, by comparison of model predictions with measurements performed in particularly critical cases, suitably selected.

In such a scenario one has to develop the capability to respond to the nuclear data demand, to a large extent, by use of theoretical and computational tools.

## 1.2. Necessity for a strong international cooperative effort.

Actually nuclear models and codes have been developed, which frequently rely on different physics, so that we are now faced with the necessity of clarifications. These may be achieved by means of a critical analysis and intercomparison of model results and particularly of model assumptions, as well as of the way they are used and coded.

This is a very necessary and important task which demands a strong international cooperative effort, as addressed by the IEC working party.

Indeed such an activity has already been initiated by means of extensive code intercomparisons, which will be a very useful starting point for the NMV activities.

## 1.3. The link to the IAEA coordinated development of a REFERENCE INPUT PARAMETER LIBRARY for nuclear data evaluation.

The number of nuclear reaction channels open increases very rapidly with projectile energy, leading to the excitation of tens or even hundreds or residual nuclei. The tremendous effort needed for input preparation makes the evaluator community appreciate the strong necessity of having available, through direct code access, reliable standard parameter libraries.

The Nuclear Data Section of the IAEA (NDS), realizing the importance of this subject matter, has started a Coordinated Research Programme (CRP) aimed at the organization of a Reference Input Parameter Library (RIPL) for nuclear model codes. Accordingly, actions will be taken on a list of 7 groups of major input parameters:

1. atomic masses and related data,
2. discrete level schemes,
3. average neutron resonance parameters,
4. optical model parameters,
5. level densities (total, partial, fission)
6. gamma-ray strength functions,
7. fission barriers.

Parameters 1,2,3 are model independent, whereas parameters 4, 5, 6, 7 are model dependent. In order to be able to decide which model parameters to be compiled, assessments achievable through critical intercomparisons of the physics underlying the different models must be made. This makes the two efforts being started by the NEANSC of OECD and by the NDS of IAEA, respectively, very much complementary, strictly interdependent, and mutually supportive. Therefore it will be one of the tasks of the s12 on NMV to provide theoretical support to the IAEA CRP on the RIPL.

## 2. NUCLEAR MODEL VALIDATION: EFFORT AND ORGANIZATION

### 2.1. The task.

The period of time in which s12 is foreseen to be active has been indicated as 3 years. It is impossible to imagine performing all the work in the physics involved up to a few hundred MeV in a 3 years time period. This period can be sufficient, however, to cast some light on the status of the art of all what may be needed in nuclear data evaluation in the energy range up to 200-300 MeV.

According to the indications of the NEANSC IEC, the NMV should consider all reaction mechanisms taking place below about one hundred MeV incident energy. One may suggest the pion production threshold as a more proper dividing line, in view of the implications of elementary particle production, a complication which requires different theoretical treatment. The energy domain so defined, typically involves reactions induced by light projectiles.

In terms of nuclear model approaches and theories currently used, the following scheme has been adopted:

SCHEMATIC REPRESENTATION OF CURRENTLY USED APPROACHES

NUCLEAR STRUCTURE	DISCRETE LEVELS REGION	SHELL MODEL & IBA HARTREE-FOCK RFA
	CONTINUUM REGION	TOTAL LVL DNST   BCS FERMI GAS SHELL MDL
		PARTIAL LVL DN   FERMI GAS SH. MDL. BCS
NUCLEAR REACTIONS	OPT. MDL & DIR. REACT.	SPHERICAL   LOCAL NON LOCAL COUPLED CH. DWBA
	R-MATRIX and R-MATRIX-SHELL MDL APP. TO LOW MASSES	
	THERMAL & RESONANCE REGION	
	COMPOUND NUCLEUS	HAUSER-FESHBACH EVAPORATIVE MDL
NUCLEAR REACTIONS	PREEQUILIBRIUM	EXCITON MODEL HYBRID MODEL FKK WEIDENMULLER ET AL. TAMURA ET AL. KALKA MODEL
	FISSION MODELS	DYNAMIC FISSION MADLAND MODEL SEELIGER MODEL
	GAMMA-RAY REACT.	G-ABSORPTION
G-PRODUCTION		COMPOUND NUCLEUS DIRECT COLLECTIVE PREEQUILIBRIUM BREMSTRAHLUNG QUASI-DEUTERON

## 2.2 The work organization.

Due to a complete lack of economical support the cooperation must take place mostly via e-mail, and this is additional good reason to split s12 into as small groups as possible.

Plenary or interdisciplinary sessions can be foreseen only at the occasion of IAEA meetings or international conferences as they arise. They will be good occasions for considering interdisciplinary aspects of links among different pieces of physics. At such occasions open problems will be raised and discussed.

From the schematic representation of table 1 one can identify at least 8 different groups of specialists. The specialists on basic theory and on evaluation which have accepted to participate into the NMV activities are grouped here below, as agreed. A reference person (underlined) has been indicated for each group.

### I. WORKING GROUP ON NUCLEAR STRUCTURE

<u>S. GRIMES</u>	(Ohio University) USA
M. HERMAN	(guest at ENEA) Italy
K. SATO	(TCPK) JAPAN
Y. NAKAJIMA	(JAERI)
A. VENTURA	(ENEA) Italy
A. V. IGNATYUK	(IPPE) Russia
SU ZONGDI	(CNDC) China
C. Y. FU	(ORNL) USA
G. ROHR	(CBNM) Belgium

### II. WORKING GROUP ON OPTICAL MODEL AND DIRECT REACTIONS

<u>F.</u>	<u>DIETRICH</u> (LLNL) USA
M. MATOBA	(KYUSHU UN.) JAPAN
K. ISHIBASHI	(KYUSHU UN.) JAPAN
Y. WATANABE	(KYUSHU UN.) JAPAN
P. G. YOUNG	(LANL) USA
V. FRONYAEV	(IPPE) Russia
B. STROHMAIER	(IRK) Austria
V. AVRIGEANU	(IPNE) Rumania
D. MADLAND	(LANL) USA
O. BERSILLON	(CEA) France

### III. WORKING GROUP ON R-MATRIX AND R-MATRIX-SHELL MODEL APPROACH FOR PARTICLE REACTIONS IN LIGHT ELEMENTS.

<u>J. HALE</u>	<u>(LANL)</u>
D. RESLER	(LLNL) USA
K. SHIBATA	(JAERI) Japan
N. LARSON	(ORNL) USA

### IV. THERMAL AND RESONANCE REGION

F. FROEHNER	(KFK) FRG
H. DERRIEN	France

V. WORKING GROUP ON COMPOUND NUCLEUS AND PREEQUILIBRIUM REACTION MECHANISMS.

M. B. CHADWICK (LLNL) USA  
P. YOUNG (LANL) USA  
M. BLANN (LLNL) USA  
C. Y. FU (ORNL) USA  
ZHANG JINGSHANG (CNDC) China  
S. CHIBA (JAERI) Japan  
Y. N. SHUBIN (IPPE) Russia  
H. WOLTER (Munchen Universitaet) FRG  
M. HERMAN (guest at ENEA) Italy  
F. DIETRICH (LLNL) USA  
A. J. KONING (ECN) HOLLAND  
H. KALKA (UNIVERSITAET DRESDEN) FRG  
Y. WATANABE (Kyushiu Univ.) Japan  
A. MARCINKOWSKI (INR) Poland  
B. STROHMAIER (IRK) AUSTRIA

VI. WORKING GROUP ON FISSION MODELS

D. MADLAND (LANL) USA  
T. OHSAWA (KINKI UN.) JAPAN  
WANG SHU NUAN (CNDC) China

VII. WORKING GROUP ON REACTION MECHANISMS INVOLVING GAMMA RAYS

M. HERMAN (guest at ENEA) Italy  
F. DIETRICH (LLNL) USA  
M. IGASHIRA (TOKYO INST. OF  
TECHN.) JA  
H. KITAZAWA (TOKYO INST. OF  
TECHN.) JA  
E. BETAK  
J. KOPECKY (ECN) Holland  
M. UHL (IRK) Austria

VIII. WORKING GROUP ON NUCLEAR MODEL INTERCOMPARISON

M. BLANN (LLNL) USA  
P. NAGEL (NEA) OCDE  
P. G. YOUNG (LANL) USA  
M. B. CHADWICK (LLNL) USA  
F. FABBRI (ENEA) Italy  
M. HERMAN (guest at ENEA) Italy  
C. Y. FU (ORNL) USA  
H. KALKA (UNIV. DRESDEN) FRG  
S. CHIBA (JAERI) Japan  
T. FUKAHORI (JAERI) JAPAN  
M. UHL (IRK) Austria  
J. A. KONING (ECN) Holland  
YU. N. SHUBIN (IPPE) RUSSIA



B. STROHMAIER (IRK) AUSTRIA  
 V. M. MASLOV (RPCPI) BELARUS  
 H. DERRIEN

### 3. CODES RECOMMENDED FOR CONSIDERATION

A list of codes has been suggested to consideration by the participants to the 1-st NMV meeting.

- |                               |   |
|-------------------------------|---|
| 1. ALICE (BLANN)              | Documented  |
| 2. GNASH (YOUNG)              | Documented  |
| 3. GNASH-FKK (YOUNG-CHADWICK) | Documented  |
| 4. STAPREH93 (AVRIGEANU)      | Documented  |
| 5. ALICE F (FUKAHORI)         |   |
| 6. SINCROS 2 (FUKAHORI-CHIBA) |   |
| 7. CATHY (FUKAHORI)           | Documented  |
| 8. ELIESE (FUKAHORI)          | Documented  |
| 9. TNG (FU)                   | Documented  |
| 10. RHOTERM (GRIMES)          | SHELL MODEL + STATISTICAL   |
| 11. EDA (HALE)                | GENERAL R-MATRIX, on Cray   |
| 12. ECIS 87 (PRONYAEV)        | Multichannel coupling   |
| 13. ECIS 94 (KONING-RAYNAL)   | Manual planned  |
| 14. EXIFON (KALKA)            | Documented  |
| 15. EXIFON C (KALKA)          |   |
| 16. CAPSIES (KONING)          |   |
| 17. GLTLTLT (MADLAND)         | Fission spectrum, average multiplicity, spectrum moment. NO DOCUMENTATION.  |
| 18. RELOMP (MADLAND)          | OPTICAL MODEL MEDIUM ENERGY SOME DOCUMENTATION  |
| 19. SNOOP 8 (MADLAND)         | SCHROEDINGER EQ. OPTICAL MODEL +RELATIVISTIC ENERGY, 2-ND ORDER DIRAC, + STANDARD OPTICAL MODEL, AS A PARTICULAR CASE |
| 20. EMPIRE (MARCINLOWSKI)     | HAUSER-FESHBACH + HYBRID. Documented.   |
| 21. EMPIRE (MARCINLOWSKI)     | + MSC FKK. Documented.  |

- |   |  |
|---|--|
| 22. ANDRE' (MARCINLOWSKI)                       | FKK-MSD . Will be documented.  |
| 23. MISDO (ROHR)                                | Level Density Calculations.  |
| 24. STAPRE (UHL)                                | COMP. NUCL. + PREEQ. EXCITON<br>MODEL, DOCUMENTED  |
| 25. FKK-GNASH (WATANABE)                        | .  |
| 26. SCIEDW (WATANABE)                           | DWBA   |
| 27. UNF (ZANG JINGSHANG)                        | EXCITON MDL, Documented.   |
| 28. FUNF (ZHANG JINGSHANG)                      | FISSILE NUCLEI   |
| 29. CUNF (ZHANG JINGSHANG)                      | CHARGED PARTICLE INDUCED REAC-<br>TIONS.   |
| 30. GUNF (ZHANG JINGSHANG)                      | GAMMA INDUCED REACTIONS.   |
| 31. IDA MODULAR SYSTEM<br>(REFFO-PABBRI-HERMAN) | AMLETO level density analysis<br>ESTIMA resonance analysis<br>ARGO reaction lists and Q-values<br>EURIALOGamma branchings<br>CERBERObinary cross sections<br>PENELOPEmultiple cascading emissions<br>NAUSICA as above + two gas preeq<br>CIRCE generalized optical model<br>EOLO valence capture<br>TELEMACO inclusive spectra calcts.<br>ULYSSES data processing. |
| 33. PEGAS (BETAK-OBLOZINSKY)                    |  |
| 34. GAMME (BONETTI-CHADWICK)                    |  |
| 35. MAURINA (UHL)                               |  |
| 36. GRAPE (GRUPPELAAR)                          |  |
| 37. SAMMY (N. LARSON)                           | R-MATRIX.  |
| 38. SCAT-2 (BERSILLON)                          | SPHERICAL OPTICAL MODEL  |
| 39. FLUKA (FERRARI et al.)                      | Documented, 1MeV-1000 GeV  |

#### 4. OBJECTIVES AND MILESTONES

The working groups are invited to produce survey-documents with comments on the experience of the group members about models and tools they have produced and/or they have been using. The existing literature can be used, only it has to be reoriented according to the needs and scope of s12 activity. These documents will be collected by the coordinator and important aspects will be brought up and will constitute discussion elements until complete agreement is reached.

Previous code intercomparisons showed how the same code may yield user-dependent results. This experience puts in evidence the necessity of special attention to the methodological aspects of nuclear modelling. We should, therefore, like to promote any effort to have (in addition to code manuals) also theory and nuclear modelling guidelines. The analysis of previous code intercomparisons will offer useful indications about which types of interpretation ambiguities have given place to different results.

Our work will proceed accordingly, aiming to the following MAIN OBJECTIVES AND MILESTONES:

- SURVEY OF THE DIFFERENT NUCLEAR MODELS DEVELOPED.  
(BY END OF '94).

This implies a thorough critical analysis and intercomparison of the physics underlying the different approaches. To this end the work done by A.J. Koning will be helpful, see document NEA/NSC/DOC(92)12.

We will have to indicate what are the advantages and drawbacks of different model approximations and to give indications, as far as possible, of the reliability of results in terms of uncertainty figures.

We should provide guidance for the correct use of the models recommended, and give comprehensive indications about model parameters and inherent systematics.

- CRITICAL INTERCOMPARISON OF MODEL CALCULATIONS AGAINST EXPERIMENT.  
(BY THE END OF '95).

Of necessity this step has to include:

- a) an assessment of the degree of confidence expected from the various approaches which will be considered.
- b) a critical intercomparison of the corresponding model codes.  
We will be greatly helped by the code intercomparison currently underway and coordinated by M. Blann and P. Nagel.  
Similarly we will have to illustrate the advantages and the range of validity of different codes considered for recommendation and release, along with user manuals.
- c) identification of critical experiments for theory testing and validation.
- d) identification of problems and gaps which may constitute the starting point of later efforts to be taken in the frame of international cooperation.

## 6. FUTURE METINGS

WE plan to have the 2-nd meeeting of s12 NMV in december 1994, by the time of the JEF-EFF meeting.

## 7. SHORT SUMMARY

++++ WHAT WE HAVE DONE AT THE FIRST s12 NMV MEETING IS:

- # AGREE ON A WORK PROGRAMME
- # AGREE ON THE ACTIONS:  
WHO IS DOING WHAT
- # AGREE ON SOME MILESTONES

++++ WHAT IS NEEDED IS:

- # OUTLINE OF BASIC PHYSICS
- # VALIDITY LIMITS
- # SUCCESS AND FAILURES
- # DIFFICULTIES
- # RANGE OF APPLICABILITY IN E AND A
- # IS THERE ANY NEED OF EXPERIMENTAL BENCHMARKING
- # DIFFERENCES FROM OTHER APPROACHES
- # PARAMETERS AND PARAMETER SYST.
- # IF MORE APPROACHES ARE AVAILABLE SELECT A FEW AND SPECIFY THE REASONS OF THE CHOICE
- # PROVIDE REFERENCES FOR DETAILS
- # IS THE APPROACH CODED
- # IS THE CODE AVAILABLE
- # IS THE CODE PROVIDED WITH MANUAL
- # ARE MORE CODES AVAILABLE
- # IS A CODE INTERCOMP. NEEDED

++++ ACTIONS

1. Reffo: send out questionnaires on codes and models by july 15.
2. Grimes: will consider level density effects on cross sections.
3. All participants: write a note on the theory-approach of interest, respectively, by the end of 1994.
4. Madland: will include folding model-dispersive approaches to optical model.
5. All participants: provide code manuals-documentation end of -94